

| Substance Name        | CASRN     | Test Lab | <i>In Vitro</i><br>Concentration<br>Tested | <i>In Vitro</i><br>Physical Form<br>Tested | Purity (%) | Solubility    | pH | IS(B) <sup>1</sup> | IS(B) SD | IS(B)<br>Classification | Overall IS(B)<br>Classification | Reference              |
|-----------------------|-----------|----------|--|--|------------|---------------|----|--------------------|----------|-------------------------|---------------------------------|------------------------|
| Acetic acid           | 64-19-7   | 2        | 100%                                       | Liquid                                     | >99        |               |    | 14.8               |          | Severe                  | Severe                          | CEC (1991)             |
| Acetic acid           | 64-19-7   | 3        | 100%                                       | Liquid                                     | >99        |               |    | 13.7               |          | Severe                  |                                 | CEC (1991)             |
| Acetic acid           | 64-19-7   | 4        | 100%                                       | Liquid                                     | >99        |               |    | 9.3                |          | Severe                  |                                 | CEC (1991)             |
| Acetic acid           | 64-19-7   | 2        | 10%  | Solution                                   | >99        |               |    | 20.2               |          | Severe                  | Severe                          | CEC (1991)             |
| Acetic acid           | 64-19-7   | 3        | 10%  | Solution                                   | >99        |               |    | 13.6               |          | Severe                  |                                 | CEC (1991)             |
| Acetic acid           | 64-19-7   | 4        | 10%  | Solution                                   | >99        |               |    | 10.2               |          | Severe                  |                                 | CEC (1991)             |
| Acetone               | 67-64-1   |          | 100%                                       | Liquid                                     | >99        | water soluble |    | 15.32              | 0.33     | Severe                  | Severe                          | Gilleron et al. (1997) |
| Allyl alcohol         | 107-18-6  |          | 100%                                       | Liquid                                     |            |               |    | 12.4               | 2.3      | Severe                  | Severe                          | Gilleron et al. (1996) |
| 2-Aminophenol         | 95-55-6   |          | 100%                                       | Solid                                      |            |               |    | 0.8                | 0.7      | Nonirritant             | Nonirritant                     | Gilleron et al. (1996) |
| Ammonium nitrate      | 6484-52-2 |          | 100%                                       | Solid                                      | >99.9      | water soluble |    | 15.34              | 1.24     | Severe                  | Severe                          | Gilleron et al. (1997) |
| Anthracene            | 120-12-7  |          | 100%                                       | Solid                                      |            |               |    | 0                  | 0        | Nonirritant             | Nonirritant                     | Gilleron et al. (1996) |
| L-Aspartic acid       | 70-47-3   |          | 100%                                       | Solid                                      | 95         | water soluble |    | 1.06               | 1.2      | Slight                  | Slight                          | Gilleron et al. (1997) |
| Benzalkonium chloride | 8001-54-5 |          | 100%                                       | Liquid                                     | 98         | surfactant    |    | 14.8               | 0.53     | Severe                  | Severe                          | Gilleron et al. (1997) |
| Benzalkonium chloride | 8001-54-5 |          | 100%                                       | Liquid                                     | 98         | surfactant    |    | 15.05              | 0.27     | Severe                  | Severe                          | Gilleron et al. (1997) |
| Benzalkonium chloride | 8001-54-5 |          | 100%                                       | Liquid                                     | 98         | surfactant    |    | 15.14              | 0.25     | Severe                  | Severe                          | Gilleron et al. (1997) |
| Benzalkonium chloride | 8001-54-5 | 2        | 100%                                       | Unknown                                    | n.p.       |               |    | 14.5               |          | Severe                  | Severe                          | CEC (1991)             |
| Benzalkonium chloride | 8001-54-5 | 3        | 100%                                       | Unknown                                    | n.p.       |               |    | 13.1               |          | Severe                  |                                 | CEC (1991)             |
| Benzalkonium chloride | 8001-54-5 | 5        | 100%                                       | Unknown                                    | n.p.       |               |    | 5.8                |          | Moderate                |                                 | CEC (1991)             |
| Benzalkonium chloride | 8001-54-5 | 6        | 100%                                       | Unknown                                    | n.p.       |               |    | 6.9                |          | Moderate                |                                 | CEC (1991)             |
| Benzalkonium chloride | 8001-54-5 | 7        | 100%                                       | Unknown                                    | n.p.       |               |    | 13.3               |          | Severe                  |                                 | CEC (1991)             |
| Benzethonium chloride | 121-54-0  |          | 100%                                       | Solid                                      | n.p.       |               |    | 15.4               | 3.1      | Severe                  | Severe                          | Gilleron et al. (1996) |

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|-----------------------|-----------|----------|--|--|------------|------------|----|--------------------|----------|-------------------------|---------------------------------|------------|
| Brij 35               | 9002-92-0 | 1        | 100%                                       | Solid                                      | >99        |            |    | 2.3                |          | Slight                  | Slight                          | CEC (1991) |
| Brij 35               | 9002-92-0 | 2        | 100%                                       | Solid                                      | >99        |            |    | 4.3                |          | Slight                  |                                 | CEC (1991) |
| Brij 35               | 9002-92-0 | 3        | 100%                                       | Solid                                      | >99        |            |    | 12.9               |          | Severe                  |                                 | CEC (1991) |
| Brij 35               | 9002-92-0 | 4        | 100%                                       | Solid                                      | >99        |            |    | 4.4                |          | Slight                  |                                 | CEC (1991) |
| Brij 35               | 9002-92-0 | 5        | 100%                                       | Solid                                      | >99        |            |    | 3.8                |          | Slight                  |                                 | CEC (1991) |
| Brij 35               | 9002-92-0 | 6        | 100%                                       | Solid                                      | >99        |            |    | 2.6                |          | Slight                  |                                 | CEC (1991) |
| Brij 35               | 9002-92-0 | 7        | 100%                                       | Solid                                      | >99        |            |    | 4                  |          | Slight                  |                                 | CEC (1991) |
| Butanol               | 71-36-3   | 1        | 100%                                       | Liquid                                     | 99         |            |    | 11.7               |          | Severe                  | Severe                          | CEC (1991) |
| Butanol               | 71-36-3   | 2        | 100%                                       | Liquid                                     | 99         |            |    | 11.8               |          | Severe                  |                                 | CEC (1991) |
| Butanol               | 71-36-3   | 3        | 100%                                       | Liquid                                     | 99         |            |    | 12.6               |          | Severe                  |                                 | CEC (1991) |
| Butanol               | 71-36-3   | 4        | 100%                                       | Liquid                                     | 99         |            |    | 11.2               |          | Severe                  |                                 | CEC (1991) |
| Butanol               | 71-36-3   | 5        | 100%                                       | Liquid                                     | 99         |            |    | 3.9                |          | Slight                  |                                 | CEC (1991) |
| Butanol               | 71-36-3   | 6        | 100%                                       | Liquid                                     | 99         |            |    | 10.7               |          | Severe                  |                                 | CEC (1991) |
| Butanol               | 71-36-3   | 7        | 100%                                       | Liquid                                     | 99         |            |    | 9.9                |          | Severe                  |                                 | CEC (1991) |
| Butanol               | 71-36-3   | 2        | 10%  | Solution                                   | 99         |            |    | 14.2               |          | Severe                  | Severe                          | CEC (1991) |
| Butanol               | 71-36-3   | 3        | 10%  | Solution                                   | 99         |            |    | 4.8                |          | Slight                  |                                 | CEC (1991) |
| Butanol               | 71-36-3   | 4        | 10%  | Solution                                   | 99         |            |    | 12.5               |          | Severe                  |                                 | CEC (1991) |
| 2-Butoxyethyl acetate | 112-07-2  | 1        | 100%                                       | Liquid                                     | 99         |            |    | 4.6                |          | Slight                  | Slight                          | CEC (1991) |
| 2-Butoxyethyl acetate | 112-07-2  | 2        | 100%                                       | Liquid                                     | 99         |            |    | 5.3                |          | Moderate                |                                 | CEC (1991) |
| 2-Butoxyethyl acetate | 112-07-2  | 3        | 100%                                       | Liquid                                     | 99         |            |    | 4.7                |          | Slight                  |                                 | CEC (1991) |
| 2-Butoxyethyl acetate | 112-07-2  | 4        | 100%                                       | Liquid                                     | 99         |            |    | 4.7                |          | Slight                  |                                 | CEC (1991) |
| 2-Butoxyethyl acetate | 112-07-2  | 5        | 100%                                       | Liquid                                     | 99         |            |    | 4                  |          | Slight                  |                                 | CEC (1991) |
| 2-Butoxyethyl acetate | 112-07-2  | 6        | 100%                                       | Liquid                                     | 99         |            |    | 3.9                |          | Slight                  |                                 | CEC (1991) |
| 2-Butoxyethyl acetate | 112-07-2  | 7        | 100%                                       | Liquid                                     | 99         |            |    | 4.5                |          | Slight                  |                                 | CEC (1991) |

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|--|-----------|----------|-------------------------------|-------------------------------|------------|-----------------|----|--------------------|----------|----------------------|------------------------------|------------------------|
| 2-Butoxyethyl acetate                  | 112-07-2  | 2        | 10%                           | Solution                      | 99         |                 |    | 4.1                |          | Slight               | Slight                       | CEC (1991)             |
| 2-Butoxyethyl acetate                  | 112-07-2  | 3        | 10%                           | Solution                      | 99         |                 |    | 0                  |          | Nonirritant          |                              | CEC (1991)             |
| 2-Butoxyethyl acetate                  | 112-07-2  | 4        | 10%                           | Solution                      | 99         |                 |    | 3.2                |          | Slight               |                              | CEC (1991)             |
| Butyl acetate                          | 123-86-4  |          | 100%                          | Liquid                        | 99         | water insoluble |    | 17.21              | 1.84     | Severe               | Severe                       | Gilleron et al. (1997) |
| Gamma-butyrolactone                    | 96-48-0   |          | 100%                          | Liquid                        |            |                 |    | 13.9               | 1.8      | Severe               | Severe                       | Gilleron et al. (1996) |
| Gamma-butyrolactone                    | 96-48-0   |          | 100%                          | Liquid                        | >99        | water soluble   |    | 19.39              | 0.83     | Severe               |                              | Gilleron et al. (1997) |
| Captan 90 concentrate                  | 133-06-2  |          | 100%                          | Solid                         | 90         | water soluble   |    | 15.07              | 0.27     | Severe               | Severe                       | Gilleron et al. (1997) |
| 4-Carboxybenzaldehyde                  | 619-66-9  |          | 100%                          | Solid                         | 95         | water insoluble |    | 3.95               | 4.69     | Slight               | Slight                       | Gilleron et al. (1997) |
| Cetylpyridinium bromide                | 140-72-7  |          | 100%                          | Liquid                        | 98         | surfactant      |    | 12.68              | 1.52     | Severe               | Severe                       | Gilleron et al. (1997) |
| Cetylpyridinium bromide                | 140-72-7  |          | 100%                          | Liquid                        | 98         | surfactant      |    | 13.53              | 2.42     | Severe               | Severe                       | Gilleron et al. (1997) |
| Cetylpyridinium bromide                | 140-72-7  |          | 100%                          | Liquid                        | 98         | surfactant      |    | 14.6               | 0.43     | Severe               | Severe                       | Gilleron et al. (1997) |
| Chlorhexidine                          | 55-56-1   |          | 100%                          | Solid                         | 99.5       | water insoluble |    | 14.87              | 3.78     | Severe               | Severe                       | Gilleron et al. (1997) |
| Cyclohexanol                           | 108-93-0  |          | 100%                          | Liquid                        | 97         | water soluble   |    | 18.96              | 0.1      | Severe               | Severe                       | Gilleron et al. (1997) |
| Cyclohexanone                          | 108-94-1  |          | 100%                          | Liquid                        |            |                 |    | 14.5               | 3.8      | Severe               | Severe                       | Gilleron et al. (1996) |
| Deoxycholic acid, sodium salt          | 302-95-4  |          | 100%                          | Solid                         |            |                 |    | 9.7                | 5.8      | Severe               | Severe                       | Gilleron et al. (1996) |
| Diacetone alcohol                      | 123-42-2  |          | 100%                          | Liquid                        |            |                 |    | 15.1               | 2.7      | Severe               | Severe                       | Gilleron et al. (1996) |
| Dibenzoyl-L-tartaric acid              | 2743-38-6 |          | 100%                          | Solid                         | np         | water soluble   |    | 13.34              | 4.24     | Severe               | Severe                       | Gilleron et al. (1997) |
| Dibenzoyl-L-tartaric acid              | 2743-38-6 |          | 100%                          | Solid                         |            |                 |    | 4.2                | 2.5      | Slight               |                              | Gilleron et al. (1996) |
| Dibenzyl phosphate                     | 1623-08-1 |          | 100%                          | Solid                         | 99.5       | water insoluble |    | 15.16              | 0.47     | Severe               | Severe                       | Gilleron et al. (1997) |
| Dibutyltin chloride                    | 683-18-1  | 1        | 100%                          | Solid                         | 97         |                 |    | 11.6               |          | Severe               | Severe                       | CEC (1991)             |
| Dibutyltin chloride                    | 683-18-1  | 2        | 100%                          | Solid                         | 97         |                 |    | 10.8               |          | Severe               |                              | CEC (1991)             |
| Dibutyltin chloride                    | 683-18-1  | 4        | 100%                          | Solid                         | 97         |                 |    | 12.6               |          | Severe               |                              | CEC (1991)             |
| Dibutyltin chloride                    | 683-18-1  | 5        | 100%                          | Solid                         | 97         |                 |    | 5.1                |          | Moderate             |                              | CEC (1991)             |
| Dibutyltin chloride                    | 683-18-1  | 6        | 100%                          | Solid                         | 97         |                 |    | 5                  |          | Moderate             |                              | CEC (1991)             |
| Dibutyltin chloride                    | 683-18-1  | 7        | 100%                          | Solid                         | 97         |                 |    | 13                 |          | Severe               |                              | CEC (1991)             |
| 2,6-Dichlorobenzoyl chloride           | 4659-45-4 |          | 100%                          | Liquid                        | 99         | water insoluble |    | 10.74              | 1.74     | Severe               | Severe                       | Gilleron et al. (1997) |
| 2,4-Dicholor-5-sulfamolyl-benzoic acid | 2736-23-4 |          | 100%                          | Solid                         |            |                 |    | 3.8                | 2.2      | Slight               | Slight                       | Gilleron et al. (1996) |
| Dimethyl biguanidine                   | 657-24-9  |          | 100%                          | Solid                         |            |                 |    | 8.4                | 2.2      | Moderate             | Moderate                     | Gilleron et al. (1996) |

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|---------------------------|------------|----------|--|--|------------|-----------------|----|--------------------|----------|-------------------------|---------------------------------|------------------------|
| 2,2-Dimethylbutanoic acid | 595-37-9   |          | 100%                                       | Liquid                                     | >99        | water insoluble |    | 15.31              | 0.24     | Severe                  | Severe                          | Gilleron et al. (1997) |
| 2,5-Dimethylhexanediol    | 110-03-2   |          | 100%                                       | Solid                                      | 99.5       | water insoluble |    | 15.33              | 0.38     | Severe                  | Severe                          | Gilleron et al. (1997) |
| Dimethyl sulfoxide        | 67-68-5    |          | 100%                                       | Liquid                                     |            |                 |    | 11.3               | 3.7      | Severe                  | Severe                          | Gilleron et al. (1996) |
| Dimethyl sulfoxide        | 67-68-5    | 1        | 100%                                       | Liquid                                     | 99.9       |                 |    | 11.7               |          | Severe                  |                                 | CEC (1991)             |
| Dimethyl sulfoxide        | 67-68-5    | 2        | 100%                                       | Liquid                                     | 99.9       |                 |    | 10.9               |          | Severe                  |                                 | CEC (1991)             |
| Dimethyl sulfoxide        | 67-68-5    | 3        | 100%                                       | Liquid                                     | 99.9       |                 |    | 11.3               |          | Severe                  |                                 | CEC (1991)             |
| Dimethyl sulfoxide        | 67-68-5    | 4        | 100%                                       | Liquid                                     | 99.9       |                 |    | 4.1                |          | Slight                  |                                 | CEC (1991)             |
| Dimethyl sulfoxide        | 67-68-5    | 5        | 100%                                       | Liquid                                     | 99.9       |                 |    | 4.9                |          | Slight                  |                                 | CEC (1991)             |
| Dimethyl sulfoxide        | 67-68-5    | 6        | 100%                                       | Liquid                                     | 99.9       |                 |    | 7.3                |          | Moderate                |                                 | CEC (1991)             |
| Dimethyl sulfoxide        | 67-68-5    | 7        | 100%                                       | Liquid                                     | 99.9       |                 |    | 11.4               |          | Severe                  |                                 | CEC (1991)             |
| Dimethyl sulfoxide        | 67-68-5    | 2        | 10%  | Solution                                   | 99.9       |                 |    | 4.4                |          | Slight                  |                                 | CEC (1991)             |
| Dimethyl sulfoxide        | 67-68-5    | 3        | 10%  | Solution                                   | 99.9       |                 |    | 4.1                |          | Slight                  |                                 | CEC (1991)             |
| Dimethyl sulfoxide        | 67-68-5    | 4        | 10%  | Solution                                   | 99.9       |                 |    | 4.1                |          | Slight                  |                                 | CEC (1991)             |
| EDTA dipotassium          | 25105-12-9 |          | 100%                                       | Solid                                      |            |                 |    | 0                  | 0        | Nonirritant             | Nonirritant                     | Gilleron et al. (1996) |
| Ethanol                   | 64-17-5    |          | 100%                                       | Liquid                                     |            |                 |    | 11.3               | 2.8      | Severe                  |                                 | Gilleron et al. (1996) |
| Ethanol                   | 64-17-5    |          | 100%                                       | Liquid                                     |            | water soluble   |    | 14.97              | 0.04     | Severe                  |                                 | Gilleron et al. (1997) |
| 2-Ethoxyethanol           | 110-80-5   |          | 100%                                       | Liquid                                     |            |                 |    | 10.5               | 2.7      | Severe                  |                                 | Gilleron et al. (1996) |
| Ethyl acetate             | 141-78-6   |          | 100%                                       | Liquid                                     | 99         | water soluble   |    | 19.32              | 0.06     | Severe                  |                                 | Gilleron et al. (1997) |
| 2-Ethyl-1-hexanol         | 104-76-7   |          | 100%                                       | Liquid                                     | 99         | water soluble   |    | 12.71              | 2.96     | Severe                  |                                 | Gilleron et al. (1997) |
| Ethyl-2-methylacetacetate | 609-14-3   |          | 100%                                       | Liquid                                     | ca. 97     | water insoluble |    | 12.94              | 2.94     | Severe                  | Severe                          | Gilleron et al. (1997) |
| Ethyl trimethyl acetate   | 3938-95-2  |          | 100%                                       | Liquid                                     | 99         | water insoluble |    | 13.82              | 2.73     | Severe                  | Severe                          | Gilleron et al. (1997) |
| Ethylacetoacetate         | 141-97-9   |          | 100%                                       | Liquid                                     |            |                 |    | 10                 | 3.2      | Severe                  | Severe                          | Gilleron et al. (1996) |
| Fomesafen                 | 72128-02-0 |          | 100%                                       | Solid                                      | 97.5       | water soluble   |    | 1.21               | 1.29     | Slight                  | Slight                          | Gilleron et al. (1997) |
| Furan                     | 110-00-9   |          | 100%                                       | Liquid                                     |            |                 |    | 5.5                | 1        | Moderate                | Moderate                        | Gilleron et al. (1996) |
| Gluconolactone            | 90-80-2    |          | 100%                                       | Solid                                      |            |                 |    | 4.6                | 3.2      | Slight                  | Slight                          | Gilleron et al. (1996) |
| DL-Glutamic acid          | 19285-83-7 |          | 100%                                       | Solid                                      |            |                 |    | 0.7                | 1.2      | Nonirritant             | Nonirritant                     | Gilleron et al. (1996) |
| Glycerol                  | 56-81-5    |          | 100%                                       | Liquid                                     | 99.5       | water soluble   |    | 14.78              | 0.75     | Severe                  | Severe                          | Gilleron et al. (1997) |

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|------------------------------------|-----------|----------|--|--|------------|-----------------|----|--------------------|----------|-------------------------|---------------------------------|------------------------|
| Glycerol                           | 56-81-5   | 1        | 100%                                       | Liquid                                     | >99        |                 |    | 10.8               |          | Severe                  | Severe                          | CEC (1991)             |
| Glycerol                           | 56-81-5   | 2        | 100%                                       | Liquid                                     | >99        |                 |    | 11.3               |          | Severe                  |                                 | CEC (1991)             |
| Glycerol                           | 56-81-5   | 3        | 100%                                       | Liquid                                     | >99        |                 |    | 10.3               |          | Severe                  |                                 | CEC (1991)             |
| Glycerol                           | 56-81-5   | 4        | 100%                                       | Liquid                                     | >99        |                 |    | 4.8                |          | Slight                  |                                 | CEC (1991)             |
| Glycerol                           | 56-81-5   | 5        | 100%                                       | Liquid                                     | >99        |                 |    | 0                  |          | Nonirritant             |                                 | CEC (1991)             |
| Glycerol                           | 56-81-5   | 6        | 100%                                       | Liquid                                     | >99        |                 |    | 0                  |          | Nonirritant             |                                 | CEC (1991)             |
| Glycerol                           | 56-81-5   | 7        | 100%                                       | Liquid                                     | >99        |                 |    | 9.4                |          | Severe                  |                                 | CEC (1991)             |
| Glycerol                           | 56-81-5   | 2        | 10%  | Solution                                   | >99        |                 |    | 8.7                |          | Moderate                | Slight                          | CEC (1991)             |
| Glycerol                           | 56-81-5   | 3        | 10%  | Solution                                   | >99        |                 |    | 4.4                |          | Slight                  |                                 | CEC (1991)             |
| Glycerol                           | 56-81-5   | 4        | 10%  | Solution                                   | >99        |                 |    | 3.6                |          | Slight                  |                                 | CEC (1991)             |
| 3-Glycidopropyltrimethoxysilane    | 2530-83-8 |          | 100%                                       | Liquid                                     |            |                 |    | 4.3                | 1        | Slight                  | Slight                          | Gilleron et al. (1996) |
| Hexadecyltrimethylammonium bromide | 57-09-0   |          | 100%                                       | Liquid                                     |            |                 |    | 10.8               | 4.8      | Severe                  | Severe                          | Gilleron et al. (1996) |
| Hexane                             | 110-54-3  |          | 100%                                       | Liquid                                     |            |                 |    | 3.1                | 2.7      | Slight                  | Slight                          | Gilleron et al. (1996) |
| n-Hexane                           | 110-54-3  | 1        | 100%                                       | Liquid                                     | 99         |                 |    | 2.9                |          | Slight                  | Slight                          | CEC (1991)             |
| n-Hexane                           | 110-54-3  | 2        | 100%                                       | Liquid                                     | 99         |                 |    | 5.4                |          | Moderate                |                                 | CEC (1991)             |
| n-Hexane                           | 110-54-3  | 3        | 100%                                       | Liquid                                     | 99         |                 |    | 4.2                |          | Slight                  |                                 | CEC (1991)             |
| n-Hexane                           | 110-54-3  | 4        | 100%                                       | Liquid                                     | 99         |                 |    | 10.3               |          | Severe                  |                                 | CEC (1991)             |
| n-Hexane                           | 110-54-3  | 5        | 100%                                       | Liquid                                     | 99         |                 |    | 2.3                |          | Slight                  |                                 | CEC (1991)             |
| n-Hexane                           | 110-54-3  | 6        | 100%                                       | Liquid                                     | 99         |                 |    | 8.1                |          | Moderate                |                                 | CEC (1991)             |
| n-Hexane                           | 110-54-3  | 7        | 100%                                       | Liquid                                     | 99         |                 |    | 2.4                |          | Slight                  |                                 | CEC (1991)             |
| n-Hexane                           | 110-54-3  | 2        | 10%  | Solution                                   | 99         |                 |    | 3.7                |          | Slight                  | Severe                          | CEC (1991)             |
| n-Hexane                           | 110-54-3  | 3        | 10%  | Solution                                   | 99         |                 |    | 0                  |          | Nonirritant             |                                 | CEC (1991)             |
| n-Hexane                           | 110-54-3  | 4        | 10%  | Solution                                   | 99         | water insoluble |    | 10.1               |          | Severe                  |                                 | CEC (1991)             |
| Hexanol                            | 111-27-3  |          | 100%                                       | Liquid                                     | 98         | water insoluble |    | 17.56              | 0.4      | Severe                  | Severe                          | Gilleron et al. (1997) |

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|--|------------|----------|-------------------------------|-------------------------------|------------|-----------------|----|--------------------|----------|----------------------|------------------------------|------------------------|
| Hydroalcoholic Formulation 1-5% Alcohol Containing   |            |          | Undiluted                     | Solution                      |            |                 |    | 4.6                |          | Slight               | Slight                       | Gettings et al. (1991) |
| Hydroalcoholic Formulation 2-10% Alcohol Containing  |            |          | Undiluted                     | Solution                      |            |                 |    | 5                  |          | Moderate             | Moderate                     | Gettings et al. (1991) |
| Hydroalcoholic Formulation 3-15% Alcohol Containing  |            |          | Undiluted                     | Solution                      |            |                 |    | 8.5                |          | Moderate             | Moderate                     | Gettings et al. (1991) |
| Hydroalcoholic Formulation 4-20% Alcohol Containing  |            |          | Undiluted                     | Solution                      |            |                 |    | 5.3                |          | Moderate             | Moderate                     | Gettings et al. (1991) |
| Hydroalcoholic Formulation 6-40% Alcohol Containing  |            |          | Undiluted                     | Solution                      |            |                 |    | 11.9               |          | Severe               | Severe                       | Gettings et al. (1991) |
| Hydroalcoholic Formulation 7-55% Alcohol Containing  |            |          | Undiluted                     | Solution                      |            |                 |    | 12.8               |          | Severe               | Severe                       | Gettings et al. (1991) |
| Hydroalcoholic Formulation 8-65% Alcohol Containing  |            |          | Undiluted                     | Solution                      |            |                 |    | 12.7               |          | Severe               | Severe                       | Gettings et al. (1991) |
| Hydroalcoholic Formulation 9-83% Alcohol Containing  |            |          | Undiluted                     | Solution                      |            |                 |    | 13.8               |          | Severe               | Severe                       | Gettings et al. (1991) |
| Hydroalcoholic Formulation 10-90% Alcohol Containing |            |          | Undiluted                     | Solution                      |            |                 |    | 13.6               |          | Severe               | Severe                       | Gettings et al. (1991) |
| Imidazole  | 288-32-4   |          | 100%                          | Solid                         |            |                 |    | 18.7               | 0.9      | Severe               | Severe                       | Gilleron et al. (1996) |
| Imidazole  | 288-32-4   |          | 100%                          | Solid                         | 99         | water soluble   |    | 19.43              | 0.49     | Severe               |                              | Gilleron et al. (1997) |
| Iminodibenzyl  | 94-19-9    |          | 100%                          | Solid                         |            |                 |    | 0                  | 0        | Nonirritant          | Nonirritant                  | Gilleron et al. (1996) |
| Isobutanol   | 78-83-1    |          | 100%                          | Liquid                        | 99.9       | water insoluble |    | 19.41              | 0.08     | Severe               | Severe                       | Gilleron et al. (1997) |
| Isopropanol  | 67-63-0    |          | 100%                          | Liquid                        | 99.9       | water soluble   |    | 14.8               | 0.21     | Severe               | Severe                       | Gilleron et al. (1997) |
| N-Lauroylsarcosine, sodium salt                      | 7631-98-3  |          | 100%                          | Solid                         |            |                 |    | 12.7               | 4.3      | Severe               | Severe                       | Gilleron et al. (1996) |
| Laurylsulfobetaine                                   | 14933-08-5 |          | 100%                          | Unknown                       |            |                 |    | 8.3                | 1.2      | Moderate             | Moderate                     | Gilleron et al. (1996) |
| Magnesium carbonate                                  | 56378-72-4 |          | 100%                          | Solid                         |            |                 |    | 1.4                | 1.9      | Slight               | Slight                       | Gilleron et al. (1996) |
| Maneb  | 12427-38-2 |          | 100%                          | Solid                         | 90         | water soluble   |    | 0.16               | 0.24     | Nonirritant          | Nonirritant                  | Gilleron et al. (1997) |
| Methanol   | 67-56-1    |          | 100%                          | Liquid                        |            |                 |    | 12.2               | 3.3      | Severe               | Severe                       | Gilleron et al. (1996) |
| 2-Methoxyethanol                                     | 109-86-4   |          | 100%                          | Liquid                        |            |                 |    | 14.5               | 0.7      | Severe               | Severe                       | Gilleron et al. (1996) |
| 2-Methoxyethanol                                     | 109-86-4   | 1        | 100%                          | Liquid                        | 99         |                 |    | 9.7                |          | Severe               | Severe                       | CEC (1991)             |
| 2-Methoxyethanol                                     | 109-86-4   | 2        | 100%                          | Liquid                        | 99         |                 |    | 12.2               |          | Severe               |                              | CEC (1991)             |
| 2-Methoxyethanol                                     | 109-86-4   | 3        | 100%                          | Liquid                        | 99         |                 |    | 12.1               |          | Severe               |                              | CEC (1991)             |
| 2-Methoxyethanol                                     | 109-86-4   | 4        | 100%                          | Liquid                        | 99         |                 |    | 8.6                |          | Moderate             |                              | CEC (1991)             |
| 2-Methoxyethanol                                     | 109-86-4   | 5        | 100%                          | Liquid                        | 99         |                 |    | 4.5                |          | Slight               |                              | CEC (1991)             |
| 2-Methoxyethanol                                     | 109-86-4   | 6        | 100%                          | Liquid                        | 99         |                 |    | 0.8                |          | Nonirritant          |                              | CEC (1991)             |
| 2-Methoxyethanol                                     | 109-86-4   | 7        | 100%                          | Liquid                        | 99         |                 |    | 3.1                |          | Slight               |                              | CEC (1991)             |

| Substance Name                      | CASRN    | Test Lab | <i>In Vitro</i><br>Concentration<br>Tested | <i>In Vitro</i><br>Physical Form<br>Tested | Purity (%) | Solubility      | pH | IS(B) <sup>1</sup> | IS(B) SD | IS(B)<br>Classification | Overall IS(B)<br>Classification | Reference              |
|-------------------------------------|----------|----------|--|--|------------|-----------------|----|--------------------|----------|-------------------------|---------------------------------|------------------------|
| 2-Methoxyethanol                    | 109-86-4 | 2        | 10%  | Solution                                   | 99         |                 |    | 7                  |          | Moderate                | Moderate                        | CEC (1991)             |
| 2-Methoxyethanol                    | 109-86-4 | 3        | 10%  | Solution                                   | 99         |                 |    | 0                  |          | Nonirritant             |                                 | CEC (1991)             |
| 2-Methoxyethanol                    | 109-86-4 | 4        | 10%  | Solution                                   | 99         |                 |    | 3.1                |          | Slight                  |                                 | CEC (1991)             |
| Methyl acetate                      | 79-20-9  |          | 100%                                       | Liquid                                     | 98         | water soluble   |    | 18.98              | 0.75     | Severe                  | Severe                          | Gilleron et al. (1997) |
| Methyl cyanoacetate                 | 105-34-0 |          | 100%                                       | Liquid                                     | 99         | water soluble   |    | 16.31              | 1.23     | Severe                  | Severe                          | Gilleron et al. (1997) |
| Methyl cyclopentane                 | 96-37-7  |          | 100%                                       | Liquid                                     | >99        | water insoluble |    | 17.14              | 1.63     | Severe                  | Severe                          | Gilleron et al. (1997) |
| Methyl ethyl ketone                 | 78-93-3  |          | 100%                                       | Liquid                                     | 99         | water soluble   |    | 18.35              | 2.52     | Severe                  | Severe                          | Gilleron et al. (1997) |
| Methyl isobutyl ketone              | 108-10-1 |          | 100%                                       | Liquid                                     | 98         | water insoluble |    | 17.75              | 2.2      | Severe                  | Severe                          | Gilleron et al. (1997) |
| Methyl isobutyl ketone              | 108-10-1 |          | 100%                                       | Liquid                                     |            |                 |    | 10.5               | 1.5      | Severe                  |                                 | Gilleron et al. (1996) |
| MYRJ 45                             |          |          | 100%                                       | Unknown                                    |            |                 |    | 0.00               | 0.00     | Nonirritant             | Nonirritant                     | Gilleron et al. (1996) |
| 1-Naphthalene acetic acid           | 86-87-3  |          | 100%                                       | Solid                                      | 99         | water soluble   |    | 7.46               | 2.37     | Moderate                | Moderate                        | Gilleron et al. (1997) |
| 1-Naphthalene acetic acid, Na salt  | 61-31-4  |          | 100%                                       | Solid                                      | 95         | water soluble   |    | 15.16              | 0.49     | Severe                  | Severe                          | Gilleron et al. (1997) |
| 1-Nitropropane                      | 108-03-2 |          | 100%                                       | Liquid                                     |            |                 |    | 2.8                | 2.7      | Slight                  | Slight                          | Gilleron et al. (1996) |
| Octanol                             | 111-87-5 |          | 100%                                       | Liquid                                     |            |                 |    | 9.8                | 1.7      | Severe                  | Severe                          | Gilleron et al. (1996) |
| Octanol                             | 111-87-5 |          | 100%                                       | Liquid                                     | >99        | water insoluble |    | 16.7               | 0.81     | Severe                  |                                 | Gilleron et al. (1997) |
| Oil/Water Emulsion-HZA              |          |          | Undiluted                                  | Solution                                   |            |                 |    | 1                  |          | Slight                  | Nonirritant                     | Gettings et al. (1994) |
| Oil/Water Emulsion-HZC              |          |          | Undiluted                                  | Solution                                   |            |                 |    | 3                  |          | Slight                  | Nonirritant                     | Gettings et al. (1994) |
| Oil/Water Emulsion-HZE              |          |          | Undiluted                                  | Solution                                   |            |                 |    | 3.67               |          | Slight                  | Nonirritant                     | Gettings et al. (1994) |
| Oil/Water Emulsion-HZF              |          |          | Undiluted                                  | Solution                                   |            |                 |    | 3.67               |          | Slight                  | Nonirritant                     | Gettings et al. (1994) |
| Oil/Water Emulsion-HZH <sup>2</sup> |          |          | Undiluted                                  | Solution                                   |            |                 |    | 23                 |          | Severe                  | Nonirritant                     | Gettings et al. (1994) |
| Oil/Water Emulsion-HZI              |          |          | Undiluted                                  | Solution                                   |            |                 |    | 0.333              |          | Nonirritant             | Nonirritant                     | Gettings et al. (1994) |
| Oil/Water Emulsion-HZJ              |          |          | Undiluted                                  | Solution                                   |            |                 |    | 3                  |          | Slight                  | Nonirritant                     | Gettings et al. (1994) |
| Oil/Water Emulsion-HZL              |          |          | Undiluted                                  | Solution                                   |            |                 |    | 10.3               |          | Severe                  | Nonirritant                     | Gettings et al. (1994) |
| Oil/Water Emulsion-HZM              |          |          | Undiluted                                  | Solution                                   |            |                 |    | 14.3               |          | Severe                  | Nonirritant                     | Gettings et al. (1994) |
| Oil/Water Emulsion-HZN              |          |          | Undiluted                                  | Solution                                   |            |                 |    | 3.67               |          | Slight                  | Nonirritant                     | Gettings et al. (1994) |
| Oil/Water Emulsion-HZO              |          |          | Undiluted                                  | Solution                                   |            |                 |    | 0                  |          | Nonirritant             | Nonirritant                     | Gettings et al. (1994) |
| Oil/Water Emulsion-HZR              |          |          | Undiluted                                  | Solution                                   |            |                 |    | 16.3               |          | Severe                  | Nonirritant                     | Gettings et al. (1994) |

| Substance Name                  | CASRN      | Test Lab | In Vitro Concentration Tested | In Vitro Physical Form Tested | Purity (%) | Solubility      | pH | IS(B) <sup>1</sup> | IS(B) SD | IS(B) Classification | Overall IS(B) Classification | Reference              |
|---------------------------------|------------|----------|-------------------------------|-------------------------------|------------|-----------------|----|--------------------|----------|----------------------|------------------------------|------------------------|
| Oil/Water Emulsion-HZS          |            |          | Undiluted                     | Solution                      |            |                 |    | 8.33               |          | Moderate             | Nonirritant                  | Gettings et al. (1994) |
| Oil/Water Emulsion-HZT          |            |          | Undiluted                     | Solution                      |            |                 |    | 1                  |          | Slight               | Nonirritant                  | Gettings et al. (1994) |
| Oil/Water Emulsion-HZU          |            |          | Undiluted                     | Solution                      |            |                 |    | 1                  |          | Slight               | Nonirritant                  | Gettings et al. (1994) |
| Oil/Water Emulsion-HZV          |            |          | Undiluted                     | Solution                      |            |                 |    | 0                  |          | Nonirritant          | Nonirritant                  | Gettings et al. (1994) |
| Oil/Water Emulsion-HZW          |            |          | Undiluted                     | Solution                      |            |                 |    | 5                  |          | Moderate             | Nonirritant                  | Gettings et al. (1994) |
| Oil/Water Emulsion-HZY          |            |          | Undiluted                     | Solution                      |            |                 |    | 9.67               |          | Severe               | Nonirritant                  | Gettings et al. (1994) |
| Parafluoraniline                | 371-40-4   |          | 100%                          | Liquid                        | 99         | water insoluble |    | 15.49              | 1.63     | Severe               | Severe                       | Gilleron et al. (1997) |
| 2,4-Pentadione                  | 123-54-6   |          | 100%                          | Liquid                        |            |                 |    | 8.8                | 3        | Moderate             | Moderate                     | Gilleron et al. (1996) |
| 1-Phenyl-3-pyrazolidine         | 92-43-3    |          | 100%                          | Solid                         |            |                 |    | 0.5                | 0.4      | Nonirritant          | Nonirritant                  | Gilleron et al. (1996) |
| Polyethylene glycol 400         | 25322-68-3 |          | 100%                          | Liquid                        |            | surfactant      |    | 14.68              | 0.55     | Severe               | Severe                       | Gilleron et al. (1997) |
| Polyoxyethylene 23 lauryl ether |            |          | 100%                          | Solid                         |            |                 |    | 1.5                | 2.6      | Slight               | Slight                       | Gilleron et al. (1996) |
| Potassium cyanate               | 590-28-3   |          | 100%                          | Solid                         | 97         | water soluble   |    | 14.27              | 1.15     | Severe               | Severe                       | Gilleron et al. (1997) |
| Promethazine HCl                | 58-33-3    |          | 100%                          | Solid                         | 98         | water soluble   |    | 6.27               | 1.41     | Moderate             | Severe                       | Gilleron et al. (1997) |
| Promethazine HCl                | 58-33-3    |          | 100%                          | Solid                         |            |                 |    | 13.9               | 2.1      | Severe               |                              | Gilleron et al. (1996) |
| Propyl-4-hydroxybenzoate        | 94-13-3    |          | 100%                          | Solid                         |            |                 |    | 1.9                | 1        | Slight               | Slight                       | Gilleron et al. (1996) |
| Pyridine                        | 110-86-1   |          | 100%                          | Liquid                        |            |                 |    | 15.8               | 3.6      | Severe               | Severe                       | Gilleron et al. (1996) |
| Pyridine                        | 110-86-1   |          | 100%                          | Liquid                        | >99        | water soluble   |    | 17.79              | 2.44     | Severe               |                              | Gilleron et al. (1997) |
| Quinacrine                      | 69-05-6    |          | 100%                          | Solid                         |            |                 |    | 6.5                | 2.2      | Moderate             | Moderate                     | Gilleron et al. (1996) |
| Quinacrine                      | 69-05-6    |          | 100%                          | Solid                         |            | water soluble   |    | 7.29               | 0.6      | Moderate             |                              | Gilleron et al. (1997) |
| Sodium lauryl sulfate           | 151-21-3   | 1        | 100%                          | Solid                         | 98         |                 |    | 11.4               |          | Severe               | Severe                       | CEC (1991)             |
| Sodium lauryl sulfate           | 151-21-3   | 2        | 100%                          | Solid                         | 98         |                 |    | 10.3               |          | Severe               |                              | CEC (1991)             |
| Sodium lauryl sulfate           | 151-21-3   | 3        | 100%                          | Solid                         | 98         |                 |    | 13.9               |          | Severe               |                              | CEC (1991)             |
| Sodium lauryl sulfate           | 151-21-3   | 4        | 100%                          | Solid                         | 98         |                 |    | 4.8                |          | Slight               |                              | CEC (1991)             |
| Sodium lauryl sulfate           | 151-21-3   | 6        | 100%                          | Solid                         | 98         |                 |    | 11.1               |          | Severe               |                              | CEC (1991)             |
| Sodium lauryl sulfate           | 151-21-3   | 7        | 100%                          | Solid                         | 98         |                 |    | 9.7                |          | Severe               |                              | CEC (1991)             |
| Sodium lauryl sulfate           | 151-21-3   | 2        | 10%                           | Solution                      | 98         |                 |    | 18.4               |          | Severe               | Severe                       | CEC (1991)             |
| Sodium lauryl sulfate           | 151-21-3   | 3        | 10%                           | Solution                      | 98         |                 |    | 14.1               |          | Severe               |                              | CEC (1991)             |
| Sodium lauryl sulfate           | 151-21-3   | 4        | 10%                           | Solution                      | 98         |                 |    | 5.1                |          | Moderate             |                              | CEC (1991)             |

| Substance Name                      | CASRN      | Test Lab | <i>In Vitro</i><br>Concentration<br>Tested | <i>In Vitro</i><br>Physical Form<br>Tested | Purity (%) | Solubility    | pH  | IS(B) <sup>1</sup> | IS(B) SD | IS(B)<br>Classification | Overall IS(B)<br>Classification | Reference                   |
|-------------------------------------|------------|----------|--|--|------------|---------------|-----|--------------------|----------|-------------------------|---------------------------------|-----------------------------|
| Sodium lauryl sulfate               | 151-21-3   |          | 1%   | Solution                                   |            |               | 3.3 | 14.22              |          | Severe                  | Nonirritant                     | Vinardell and Macián (1994) |
| Sodium lauryl sulfate               | 151-21-3   |          | 100%                                       | Liquid                                     | 98         | surfactant    |     | 12.38              | 1.82     | Severe                  | Severe                          | Gilleron et al. (1997)      |
| Sodium lauryl sulfate               | 151-21-3   |          | 100%                                       | Liquid                                     | 98         | surfactant    |     | 15.05              | 0.29     | Severe                  | Severe                          | Gilleron et al. (1997)      |
| Sodium hydroxide                    | 1310-73-2  |          | 100%                                       | Liquid                                     |            | water soluble |     | 19.01              | 0.13     | Severe                  | Severe                          | Gilleron et al. (1997)      |
| Sodium hydroxide                    | 1310-73-2  |          | 100%                                       | Liquid                                     |            | water soluble |     | 20.56              | 0.08     | Severe                  | Severe                          | Gilleron et al. (1997)      |
| Sodium oxalate                      | 62-76-0    |          | 100%                                       | Solid                                      | >99        | water soluble |     | 14.2               | 0.71     | Severe                  | Severe                          | Gilleron et al. (1997)      |
| Sodium perborate                    | 10486-00-7 |          | 100%                                       | Solid                                      | 98.6       | water soluble |     | 13.19              | 1.78     | Severe                  | Severe                          | Gilleron et al. (1997)      |
| Surfactant Based Formulation 1-HZA  |            |          | 10%  | Solution                                   |            |               |     | 9.6                |          | Severe                  | Nonirritant                     | Gettings et al. (1996)      |
| Surfactant Based Formulation 2-HZB  |            |          | 10%  | Solution                                   |            |               |     | 7.3                |          | Moderate                | Nonirritant                     | Gettings et al. (1996)      |
| Surfactant Based Formulation 3-HZC  |            |          | 10%  | Solution                                   |            |               |     | 15.3               |          | Severe                  | Nonirritant                     | Gettings et al. (1996)      |
| Surfactant Based Formulation 4-HZD  |            |          | 10%  | Solution                                   |            |               |     | 8.7                |          | Moderate                | Nonirritant                     | Gettings et al. (1996)      |
| Surfactant Based Formulation 5-HZE  |            |          | 10%  | Solution                                   |            |               |     | 11.4               |          | Severe                  | Nonirritant                     | Gettings et al. (1996)      |
| Surfactant Based Formulation 6-HZF  |            |          | 10%  | Solution                                   |            |               |     | 10.9               |          | Severe                  | Nonirritant                     | Gettings et al. (1996)      |
| Surfactant Based Formulation 7-HZG  |            |          | 10%  | Solution                                   |            |               |     | 7.1                |          | Moderate                | Nonirritant                     | Gettings et al. (1996)      |
| Surfactant Based Formulation 8-HZH  |            |          | 10%  | Solution                                   |            |               |     | 3.5                |          | Slight                  | Nonirritant                     | Gettings et al. (1996)      |
| Surfactant Based Formulation 9-HZI  |            |          | 10%  | Solution                                   |            |               |     | 15.2               |          | Severe                  | Nonirritant                     | Gettings et al. (1996)      |
| Surfactant Based Formulation 10-HZJ |            |          | 10%  | Solution                                   |            |               |     | 6.2                |          | Moderate                | Nonirritant                     | Gettings et al. (1996)      |
| Surfactant Based Formulation 11-HZK |            |          | 10%  | Solution                                   |            |               |     | 9.4                |          | Severe                  | Nonirritant                     | Gettings et al. (1996)      |
| Surfactant Based Formulation 12-HZL |            |          | 10%  | Solution                                   |            |               |     | 12.4               |          | Severe                  | Nonirritant                     | Gettings et al. (1996)      |
| Surfactant Based Formulation 13-HZM |            |          | 10%  | Solution                                   |            |               |     | 2.7                |          | Slight                  | Nonirritant                     | Gettings et al. (1996)      |
| Surfactant Based Formulation 14-HZN |            |          | 10%  | Solution                                   |            |               |     | 8                  |          | Moderate                | Nonirritant                     | Gettings et al. (1996)      |
| Surfactant Based Formulation 15-HZP |            |          | 10%  | Solution                                   |            |               |     | 4.4                |          | Slight                  | Nonirritant                     | Gettings et al. (1996)      |
| Surfactant Based Formulation 16-HZQ |            |          | 10%  | Solution                                   |            |               |     | 4.2                |          | Slight                  | Nonirritant                     | Gettings et al. (1996)      |
| Surfactant Based Formulation 17-HZR |            |          | 10%  | Solution                                   |            |               |     | 5.3                |          | Moderate                | Nonirritant                     | Gettings et al. (1996)      |
| Surfactant Based Formulation 18-HZS |            |          | 10%  | Solution                                   |            |               |     | 12.2               |          | Severe                  | Nonirritant                     | Gettings et al. (1996)      |
| Surfactant Based Formulation 19-HZT |            |          | 10%  | Solution                                   |            |               |     | 3.5                |          | Slight                  | Nonirritant                     | Gettings et al. (1996)      |
| Surfactant Based Formulation 20-HZU |            |          | 10%  | Solution                                   |            |               |     | 6.2                |          | Moderate                | Nonirritant                     | Gettings et al. (1996)      |

| Substance Name                      | CASRN     | Test Lab | In Vitro Concentration Tested | In Vitro Physical Form Tested | Purity (%) | Solubility      | pH | IS(B) <sup>1</sup> | IS(B) SD | IS(B) Classification | Overall IS(B) Classification | Reference              |
|-------------------------------------|-----------|----------|-------------------------------|-------------------------------|------------|-----------------|----|--------------------|----------|----------------------|------------------------------|------------------------|
| Surfactant Based Formulation 21-HZV |           |          | 10%                           | Solution                      |            |                 |    | 8.7                |          | Moderate             | Nonirritant                  | Gettings et al. (1996) |
| Surfactant Based Formulation 22-HZW |           |          | 10%                           | Solution                      |            |                 |    | 5.1                |          | Moderate             | Nonirritant                  | Gettings et al. (1996) |
| Surfactant Based Formulation 23-HZX |           |          | 10%                           | Solution                      |            |                 |    | 11.3               |          | Severe               | Nonirritant                  | Gettings et al. (1996) |
| Surfactant Based Formulation 24-HZY |           |          | 10%                           | Solution                      |            |                 |    | 11.7               |          | Severe               | Nonirritant                  | Gettings et al. (1996) |
| Surfactant Based Formulation 25-HZZ |           |          | 10%                           | Solution                      |            |                 |    | 1.1                |          | Slight               | Nonirritant                  | Gettings et al. (1996) |
| Tetraaminopyrimidine sulfate        | 5392-28-9 |          | 100%                          | Solid                         |            |                 |    | 0.5                | 0.9      | Nonirritant          | Slight                       | Gilleron et al. (1996) |
| Tetraaminopyrimidine sulfate        | 5392-28-9 |          | 100%                          | Solid                         | 97         | water insoluble |    | 4.33               | 0.23     | Slight               |                              | Gilleron et al. (1997) |
| Thiourea                            | 62-56-6   |          | 100%                          | Solid                         |            |                 |    | 13.7               | 4.4      | Severe               | Severe                       | Gilleron et al. (1996) |
| Thiourea                            | 62-56-6   |          | 100%                          | Solid                         | >99        | water soluble   |    | 17.89              | 1.53     | Severe               |                              | Gilleron et al. (1997) |
| Toluene                             | 108-88-3  |          | 100%                          | Liquid                        | 99         | water soluble   |    | 16.09              | 1.62     | Severe               | Severe                       | Gilleron et al. (1997) |
| Toluene                             | 108-88-3  | 1        | 100%                          | Liquid                        | 99.9       |                 |    | 8.8                |          | Moderate             | Severe                       | CEC (1991)             |
| Toluene                             | 108-88-3  | 2        | 100%                          | Liquid                        | 99.9       |                 |    | 14.8               |          | Severe               |                              | CEC (1991)             |
| Toluene                             | 108-88-3  | 3        | 100%                          | Liquid                        | 99.9       |                 |    | 15.2               |          | Severe               |                              | CEC (1991)             |
| Toluene                             | 108-88-3  | 4        | 100%                          | Liquid                        | 99.9       |                 |    | 11.5               |          | Severe               |                              | CEC (1991)             |
| Toluene                             | 108-88-3  | 5        | 100%                          | Liquid                        | 99.9       |                 |    | 4.6                |          | Slight               |                              | CEC (1991)             |
| Toluene                             | 108-88-3  | 6        | 100%                          | Liquid                        | 99.9       |                 |    | 3.1                |          | Slight               |                              | CEC (1991)             |
| Toluene                             | 108-88-3  | 7        | 100%                          | Liquid                        | 99.9       |                 |    | 4.9                |          | Slight               |                              | CEC (1991)             |
| Triacetin                           | 102-76-1  | 1        | 100%                          | Liquid                        | 99         |                 |    | 3.6                |          | Slight               | Slight                       | CEC (1991)             |
| Triacetin                           | 102-76-1  | 2        | 100%                          | Liquid                        | 99         |                 |    | 4.3                |          | Slight               |                              | CEC (1991)             |
| Triacetin                           | 102-76-1  | 3        | 100%                          | Liquid                        | 99         |                 |    | 5.5                |          | Moderate             |                              | CEC (1991)             |
| Triacetin                           | 102-76-1  | 4        | 100%                          | Liquid                        | 99         |                 |    | 4.4                |          | Slight               |                              | CEC (1991)             |
| Triacetin                           | 102-76-1  | 5        | 100%                          | Liquid                        | 99         |                 |    | 3.3                |          | Slight               |                              | CEC (1991)             |
| Triacetin                           | 102-76-1  | 6        | 100%                          | Liquid                        | 99         |                 |    | 4.3                |          | Slight               |                              | CEC (1991)             |
| Triacetin                           | 102-76-1  | 7        | 100%                          | Liquid                        | 99         |                 |    | 3.1                |          | Slight               |                              | CEC (1991)             |

| Substance Name         | CASRN     | Test Lab | <i>In Vitro</i><br>Concentration<br>Tested | <i>In Vitro</i><br>Physical Form<br>Tested | Purity (%) | Solubility    | pH | IS(B) <sup>1</sup> | IS(B) SD | IS(B)<br>Classification | Overall IS(B)<br>Classification | Reference              |
|------------------------|-----------|----------|--|--|------------|---------------|----|--------------------|----------|-------------------------|---------------------------------|------------------------|
| Triacetin              | 102-76-1  | 2        | 10%  | Solution                                   | 99         |               |    | 13.6               |          | Severe                  | Slight                          | CEC (1991)             |
| Triacetin              | 102-76-1  | 3        | 10%  | Solution                                   | 99         |               |    | 2                  |          | Slight                  |                                 | CEC (1991)             |
| Triacetin              | 102-76-1  | 4        | 10%  | Solution                                   | 99         |               |    | 3.3                |          | Slight                  |                                 | CEC (1991)             |
| Tributyltin chloride   | 1461-22-9 | 1        | 100%                                       | Solid                                      | 96         |               |    | 6.7                |          | Moderate                | Moderate                        | CEC (1991)             |
| Tributyltin chloride   | 1461-22-9 | 2        | 100%                                       | Solid                                      | 96         |               |    | 8.9                |          | Moderate                |                                 | CEC (1991)             |
| Tributyltin chloride   | 1461-22-9 | 3        | 100%                                       | Solid                                      | 96         |               |    | 13.7               |          | Severe                  |                                 | CEC (1991)             |
| Tributyltin chloride   | 1461-22-9 | 4        | 100%                                       | Solid                                      | 96         |               |    | 8.8                |          | Moderate                |                                 | CEC (1991)             |
| Tributyltin chloride   | 1461-22-9 | 5        | 100%                                       | Solid                                      | 96         |               |    | 7.4                |          | Moderate                |                                 | CEC (1991)             |
| Tributyltin chloride   | 1461-22-9 | 6        | 100%                                       | Solid                                      | 96         |               |    | 7.9                |          | Moderate                |                                 | CEC (1991)             |
| Tributyltin chloride   | 1461-22-9 | 7        | 100%                                       | Solid                                      | 96         |               |    | 6.6                |          | Moderate                |                                 | CEC (1991)             |
| Tributyltin chloride   | 1461-22-9 | 2        | 10%  | Solution                                   | 96         |               |    | 15.6               |          | Severe                  |                                 | CEC (1991)             |
| Tributyltin chloride   | 1461-22-9 | 3        | 10%  | Solution                                   | 96         |               |    | 9.6                |          | Severe                  | Severe                          | CEC (1991)             |
| Tributyltin chloride   | 1461-22-9 | 4        | 10%  | Solution                                   | 96         |               |    | 11.2               |          | Severe                  |                                 | CEC (1991)             |
| Trichloroacetic acid   | 76-03-9   |          | 100%                                       | Liquid                                     |            | water soluble |    | 15.7               | 0.11     | Severe                  |                                 | Gilleron et al. (1997) |
| Trichloroacetic acid   | 76-03-9   |          | 100%                                       | Liquid                                     |            | water soluble |    | 15.72              | 0.15     | Severe                  | Severe                          | Gilleron et al. (1997) |
| 1,2,3-Trichloropropane | 96-18-4   |          | 100%                                       | Liquid                                     |            |               |    | 7.9                | 1.7      | Moderate                |                                 | Gilleron et al. (1996) |
| 1,2,4-Trichloropropane | 95-63-6   |          | 100%                                       | Liquid                                     |            |               |    | 4.5                | 2.9      | Slight                  | Severe                          | Gilleron et al. (1996) |
| Triethanolamine        | 102-71-6  |          | 100%                                       | Liquid                                     |            |               |    | 9.6                | 3.5      | Severe                  |                                 | Gilleron et al. (1996) |
| Triethanolamine        | 102-71-6  | 1        | 100%                                       | Liquid                                     | 97         |               |    | 8.6                |          | Moderate                | Severe                          | CEC (1991)             |
| Triethanolamine        | 102-71-6  | 2        | 100%                                       | Liquid                                     | 97         |               |    | 10.4               |          | Severe                  |                                 | CEC (1991)             |
| Triethanolamine        | 102-71-6  | 3        | 100%                                       | Liquid                                     | 97         |               |    | 11.9               |          | Severe                  |                                 | CEC (1991)             |
| Triethanolamine        | 102-71-6  | 4        | 100%                                       | Liquid                                     | 97         |               |    | 4.2                |          | Slight                  |                                 | CEC (1991)             |
| Triethanolamine        | 102-71-6  | 5        | 100%                                       | Liquid                                     | 97         |               |    | 0                  |          | Nonirritant             |                                 | CEC (1991)             |
| Triethanolamine        | 102-71-6  | 6        | 100%                                       | Liquid                                     | 97         |               |    | 3.7                |          | Slight                  | Severe                          | CEC (1991)             |
| Triethanolamine        | 102-71-6  | 7        | 100%                                       | Liquid                                     | 97         |               |    | 7.5                |          | Moderate                |                                 | CEC (1991)             |

| Substance Name  | CASRN     | Test Lab | In Vitro Concentration Tested | In Vitro Physical Form Tested | Purity (%) | Solubility | pH   | IS(B) <sup>1</sup> | IS(B) SD | IS(B) Classification | Overall IS(B) Classification | Reference                   |
|-----------------|-----------|----------|-------------------------------|-------------------------------|------------|------------|------|--------------------|----------|----------------------|------------------------------|-----------------------------|
| Triethanolamine | 102-71-6  | 2        | 10%                           | Solution                      | 97         |            |      | 11.3               |          | Severe               | Slight                       | CEC (1991)                  |
| Triethanolamine | 102-71-6  | 3        | 10%                           | Solution                      | 97         |            |      | 2.8                |          | Slight               |                              | CEC (1991)                  |
| Triethanolamine | 102-71-6  | 4        | 10%                           | Solution                      | 97         |            |      | 1.1                |          | Slight               |                              | CEC (1991)                  |
| Triton X-100    | 9002-93-1 |          | 100%                          | Liquid                        | 98         | surfactant |      | 10.94              | 0.8      | Severe               | Severe                       | Gilleron et al. (1997)      |
| Triton X-100    | 9002-93-1 |          | 100%                          | Liquid                        | 98         | surfactant |      | 13.73              | 0.48     | Severe               | Severe                       | Gilleron et al. (1997)      |
| Triton X-155    | 9010-44-0 |          | 100%                          | Surfactant                    |            |            |      | 3.9                | 2.3      | Slight               | Slight                       | Gilleron et al. (1996)      |
| Tween 20        | 9005-64-5 |          | 100%                          | Liquid                        | 98         | surfactant |      | 14.47              | 0.36     | Severe               | Severe                       | Gilleron et al. (1997)      |
| Tween 20        | 9005-64-5 |          | 100%                          | Liquid                        |            |            | 7.21 | 3.22               |          | Slight               |                              | Vinardell and Macián (1994) |

Abbreviation: CASRN = Chemical Abstract Service Registry Number, SD = standard deviation.

<sup>1</sup> IS(B) represents irritation scores that were calculated using a method similar to the one described in Kalweit et al. (1987, 1990).

<sup>2</sup> The IS(B) analysis method does not yield an IS value greater than 21 and the calculated result of 23 for this substance is not possible. Based on results with the IS(A) analysis method (IS(A) = 17.8) in the same report, the formulation would be classified as a severe irritant and was classified as such for the IS(B) analysis method.